

# Phase coherence and “fragmented” Bose condensates

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submitted November 27, 1998; PACS 03.75 Fi

**We show that a “fragmented Bose condensate” in which two or more distinct single-particle states are macroscopically occupied by the same species of boson is inherently unstable to the formation of a conventional Bose condensate whose macroscopically occupied state is a linear combination of the “fragments” with definite relative phases. A related analysis shows that a reproducible relative phase develops when two initially decoupled condensates are placed in contact.**

The essential property of a Bose condensate is the existence of a single macroscopically large eigenvalue of its one-body density matrix.<sup>1-3</sup> This property reveals the existence of long-range phase coherence across the fluid, which leads to the two-fluid description of Bose condensates and implies the quantization of circulation in superfluid flow.<sup>4,5</sup> Hypothetical Bose states without this property were discussed long ago by Nozieres and St. James<sup>6,7</sup>, and have recently received renewed theoretical attention in the case of trapped bosons.<sup>8,9</sup> In particular, Wilkin *et al.*<sup>8</sup> found that the azimuthally symmetric rotating states of a dilute Bose gas with attractive interactions are “fragmented” Bose condensates in which many single-particle states (of differing angular momenta) are macroscopically occupied. Such multi-condensate Bose fluids would be expected to have unusual properties.

A related set of issues stems from a *gedankenexperiment* proposed by Anderson,<sup>10</sup> in which two previously isolated Bose condensates are brought into particle-exchanging contact. Before contact is initiated, each isolated subsystem has its own macroscopically occupied state. The two isolated Bose subsystems considered together therefore provide a simple example of a system with a “fragmented” condensate. What happens when the condensates are allowed to exchange particles – will the phase difference be random from experiment to experiment,<sup>10,13,14</sup> or be reproducibly zero<sup>11,12</sup>?

Here we show that when fragmented condensates overlap, they are inherently unstable to the formation of a single, conventional condensate of well-defined relative phase. The essential idea is that even weak Josephson coupling between the fragments rapidly generates phase coherence, modifying the density matrix deterministically to give a unique macroscopically occupied single particle state. The proof proceeds by first assuming the existence of a Bose state with multiple condensates, and then explicitly constructing a lower energy state. The

argument is very general, and applies to strongly as well as weakly interacting systems, and for either sign of the scattering length. As a corollary, we show that the relative phase that emerges when two previously uncoupled condensates are placed in contact is reproducible, and is determined by the physics of coherent particle exchange between them.

**Multiple condensates.** Consider a fluid of  $N$  identical Bose particles. Let  $|0\rangle$  be a many-body state that is presumed to be both (a) the ground state of a many-body Hamiltonian  $\mathcal{H}$  and (b) a “fragmented condensate,” *i.e.*, a state whose reduced one-body density matrix

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \langle \hat{\psi}(\mathbf{r}')^\dagger \hat{\psi}(\mathbf{r}) \rangle \quad (1)$$

has two or more macroscopic eigenvalues  $N_i$ , with corresponding eigenfunctions  $\phi_i(\mathbf{r})$ . The  $N_i$  have the physical interpretation of the mean occupancy of the single-particle state  $\phi_i$  in the many-body state  $|0\rangle$ . In general the macroscopic  $N_i$  are not integers, and they need not add up to the total particle number  $N$ . For simplicity, we will assume that only two such macroscopic eigenvalues exist, but our arguments are easily generalized to any finite number.<sup>24</sup>

We define the condensate annihilation operators

$$b_i \equiv \int d\mathbf{r} \phi_i(\mathbf{r}) \hat{\psi}(\mathbf{r}) \quad (2)$$

where  $\hat{\psi}(\mathbf{r})$  is the particle annihilation operator at position  $\mathbf{r}$ . Then in the fragmented state,

$$[\hat{\rho}_0]_{ij} = \langle 0 | b_j^\dagger b_i | 0 \rangle = N_i \delta_{ij}, \quad (3)$$

which follows from the assumption that  $\phi_i$  are eigenstates of  $\hat{\rho}$ . For  $i \neq j$  the density matrix element vanishes, indicating the absence of coherence between the condensates.

**A family of states.** We now construct a family of  $N$ -particle states labeled by the integers  $q = 0, \pm 1, \pm 2, \dots$  in which  $q$  particles are transferred between the two condensates. For positive  $q$ , the transfer is from 1 to 2; for negative  $q$ , the transfer is from 2 to 1; the  $q = 0$  state is simply the original fragmented state  $|0\rangle$ . These states can be formed by repeated applications of the operator

$$B^\dagger \equiv \frac{b_2^\dagger b_1}{\sqrt{N_2 N_1}} \quad (4)$$

for positive  $q$ , and its Hermitian conjugate  $B$  for negative  $q$ . The factors in the denominator make the states

$$|q\rangle \equiv (B^\dagger)^q |0\rangle \quad q \geq 0 \quad (5)$$

$$|q\rangle \equiv (B)^{|q|} |0\rangle \quad q < 0 \quad (6)$$

normalized for  $q \ll N_i$ , which will be the case of interest below. The operator  $\hat{Q}$  can then be defined as  $\sum q |q\rangle \langle q|$ . Our strategy will be to construct a linear combination of the states  $|q\rangle$  that is lower in energy than the putative ground state  $|0\rangle$ .

**An effective tight-binding model.** We consider a many-body Hamiltonian  $\mathcal{H}$  given by the sum of a one-body part  $\hat{h}_o$  – kinetic energy plus a single-particle potential  $V(\mathbf{r})$  – and a two-body interaction  $U(\mathbf{r}-\mathbf{r}')$ , which for notational simplicity we will take to be a  $\delta$ -function pseudopotential of strength  $U$ . (Our results are easily extended to more general interactions.) Within the subspace of states  $\{|q\rangle\}$ ,  $\mathcal{H}$  can be written

$$\mathcal{H} = -[t_1 B^\dagger + t_1^* B] - [t_2 (B^\dagger)^2 + t_2^* B^2] + \frac{1}{2} \kappa Q^2, \quad (7)$$

which has the form of a one-dimensional tight-binding model with nearest and next-nearest neighbor hopping matrix elements  $t_1$  and  $t_2$ , and a harmonic potential of spring constant  $\kappa$ .

The generally complex hopping matrix elements are given by

$$t_1 = -\sqrt{N_1 N_2} \int d\mathbf{r} \phi_2^*(\mathbf{r}) \hat{h}_{\text{eff}} \phi_1(\mathbf{r}), \quad (8)$$

$$t_2 = -\frac{U}{2} N_1 N_2 \int d\mathbf{r} \phi_2^*(\mathbf{r}) \phi_2^*(\mathbf{r}) \phi_1(\mathbf{r}) \phi_1(\mathbf{r}), \quad (9)$$

where  $\hat{h}_{\text{eff}} \equiv \hat{h}_o + U \sum_i N_i |\phi_i(\mathbf{r})|^2$  is an effective one-body Hamiltonian that includes mean field interactions.

If the condensates  $\phi_i(\mathbf{r})$  extend over the same  $d$ -dimensional volume  $R^d$ , where  $R$  is a characteristic length scale, then the matrix elements of eq. (89) scale as  $t_1 \sim N\epsilon_1$  and  $t_2 \sim N\epsilon_2$ , where the  $\epsilon_i$  are functions of the mean density  $N/R^d$  with the units of energy per particle. Typically, they will be of the same order of magnitude as the chemical potential.<sup>25</sup> We consider below the special case in which the matrix elements  $t_1$  and  $t_2$  vanish for symmetry reasons.

The hopping terms of the Hamiltonian (7) give rise to a tight-binding band with dispersion

$$E(k) = -[t_1 e^{-ik} + t_1^* e^{ik}] - [t_2 e^{-i2k} + t_2^* e^{i2k}], \quad (10)$$

which can be expanded about its minimum to yield

$$E(k) = -\frac{TN}{2} + \frac{T'N}{2}(k - \chi)^2 + \dots \quad (11)$$

where the real numbers  $T$  and  $T'$  depend on the  $\epsilon_i$ , and  $\chi$  can be found by minimizing eq. (10). The effective mass for this band is given by  $\hbar^2/M_{\text{eff}} = T'N$ .

The “spring constant”  $\kappa$  in eq. (7) can be found quite generally from the assumption that the condensates are compressible, which is expected on general grounds for a Bose fluid.<sup>26</sup> Then the energy of a state with  $q_i$  particles added to condensate  $i$  (by repeated application of  $b_i^\dagger$ ) will be a smooth function that can be Taylor expanded for small  $q_i \ll N_i$ , so that

$$\langle q | \mathcal{H} | q \rangle = E_0 + q(\mu_1 - \mu_2) + \frac{\kappa}{2} q^2 + \dots \quad (12)$$

where  $\mu_i \equiv \partial E / \partial N_i$  is the chemical potential of the  $i$ -th fragment and

$$\kappa = \frac{K}{N} \equiv \left[ \frac{\partial^2 E}{\partial N_1^2} - 2 \frac{\partial^2 E}{\partial N_1 \partial N_2} + \frac{\partial^2 E}{\partial N_2^2} \right]. \quad (13)$$

For condensates  $\phi_i$  of volume  $R^d$ ,  $K$  is a number of order  $U(N/R^d)$  that is again comparable to the chemical potential, and hence  $T$  and  $T'$ . Since by assumption  $q = 0$  is the ground state the chemical potentials must be equal and the linear term in  $q$  vanishes. For stability,  $\kappa$  must be positive.

The tight-binding model (7) for two coupled condensates is related by a canonical transformation to the familiar pendulum description of a Josephson junction,<sup>19</sup> which treats the relative phase as a periodic “coordinate” and the number fluctuation as its corresponding “momentum.” The present analysis instead takes the number fluctuation as a discrete coordinate, with relative phase corresponding to the conjugate (crystal) momentum. The two approaches are completely equivalent, and provide complementary insights to the behavior of coupled condensates.

**A lower energy state.** Within a continuum approximation, the tight-binding Hamiltonian (7) describes a particle of mass  $M_{\text{eff}}$  in a harmonic potential of spring constant  $\kappa$ . The frequency of this oscillator is given by  $M_{\text{eff}} \omega_{\text{eff}}^2 = \kappa$ , so that  $\hbar \omega_{\text{eff}} = \sqrt{T'K}$ . The ground state has the form

$$|G\rangle = \sum_q \frac{e^{-q^2/2\sigma^2}}{\pi^{1/4} \sigma^{1/2}} e^{i\chi q} |q\rangle, \quad (14)$$

with a characteristic spread in  $q$

$$\sigma = (\hbar/M_{\text{eff}} \omega_{\text{eff}})^{1/2} = (T'/K)^{1/4} N^{1/2}. \quad (15)$$

Since  $\sigma \sim N^{1/2}$ , we are justified *a posteriori* in both the continuum approximation and our decision to neglect terms of order  $q^3$  (and higher) in  $E(q)$ .

The energy of  $|G\rangle$  relative to  $|0\rangle$  is

$$E_G - E_0 = -\frac{TN}{2} + \frac{(T'K)^{1/2}}{2}, \quad (16)$$

where the first term on the right is the delocalization energy of the bottom of the tight-binding band, and the second is the zero-point energy of a harmonic oscillator with energy spacing  $\hbar \omega_{\text{eff}}$ . Evidently the admixture of correlated condensate fluctuations  $|G\rangle$  is lower in energy than the fragmented state  $|q = 0\rangle$  if  $N > T'K/(T^2)$ , where the right hand side is of order unity.<sup>27</sup> Thus even for extremely weak off-diagonal couplings, a fragmented condensate will not be the ground state for a macroscopic number of particles.

**Density matrix revisited.** What is the nature of the true ground state  $|G\rangle$ ? It is easy to show that  $|G\rangle$  is, in fact, a conventional Bose condensate whose density matrix has a *unique* macroscopic eigenvalue. Since  $q \ll N_i$ , the diagonal matrix elements of  $\hat{\rho}$  are unchanged

$$[\hat{\rho}_G]_{ii} = \langle G | b_i^\dagger b_i | G \rangle = N_i. \quad (17)$$

The off-diagonal matrix elements, however, are now macroscopic:

$$[\hat{\rho}_G]_{12} = \langle G | b_2^\dagger b_1 | G \rangle = g e^{-i\chi} \sqrt{N_1 N_2} \quad (18)$$

where

$$g = e^{-1/4\sigma^2} \approx 1 - \frac{A}{N}, \quad (19)$$

where  $A$  is a number of order unity.

Rediagonalizing the density matrix, we find a *single* macroscopically occupied eigenstate

$$\phi_g(\mathbf{r}) = c_1 \phi_1(\mathbf{r}) + e^{i\chi} c_2 \phi_2(\mathbf{r}), \quad (20)$$

where  $c_i \equiv \sqrt{N_i/[N_1 + N_2]}$ . The occupation of this state is  $N_g = N_1 + N_2 - B$ , where  $B$  is proportional to  $A$ , and is also a number of order unity. The orthogonal combination  $\phi_-(\mathbf{r}) = c_2 \phi_1(\mathbf{r}) - e^{i\chi} c_1 \phi_2(\mathbf{r})$  has eigenvalue  $B$  of order unity. We conclude that fragmented condensates are unstable towards the formation of conventional Bose condensate with a unique macroscopically occupied state.

**Spontaneous symmetry breaking.** As noted above, the matrix elements  $t_i$  may vanish for symmetry reasons. As a specific example, consider a rotationally invariant system with two fragments  $\phi_1$  and  $\phi_2$  that have angular momentum projections  $m_1$ ,  $m_2$ , respectively. Then the  $t_i$  will be zero. This situation arises in the context of rotating Bose gases trapped in an azimuthally symmetric potential.<sup>8</sup> Under these circumstances, we must ask if the fragmented condensate remains stable in the presence of a small symmetry-breaking perturbation, which introduces a nonzero  $t_1$ .

We have seen, however, that even for  $T \sim 1/N^2$  a fragmented condensate will be unstable to the formation of a conventional condensate (20) that is a superposition of the fragments, with a relative phase  $\chi$  that is determined by the details of the perturbing potential through eq. (8). The resulting state is not an eigenstate of angular momentum, and therefore has an asymmetric density and current distribution.<sup>17</sup> The fact that an order  $1/N$  perturbation can reduce the symmetry of the ground state indicates that fragmented condensates will spontaneously break whatever symmetry (rotation, in the case of ref. 8) permitted fragmentation in the first place.

This result can be understood in another way by considering the susceptibility of a fragmented condensate to a perturbation which couples to the inter-fragment current density  $\hat{J} \equiv i[t_1 B^\dagger - t_1^* B]$ . Since  $\langle (B^\dagger)^2 \rangle = \langle B^2 \rangle = 0$  in the  $q = 0$  state, while  $B^\dagger B = B B^\dagger = 1$  as an operator identity, the mean-square current fluctuation  $\langle J^2 \rangle \sim |t_1|^2$ . A weak one-body potential that allows scattering between  $\phi_1$  and  $\phi_2$ , however, will typically introduce a  $t_1 \sim N$ . Fragmented condensates are thus highly susceptible to perturbations that permit coherent particle transfer between the fragments.

**Gauge covariance.** The phase factor  $e^{i\chi}$  which enters into the superposition (20) is not arbitrary, but is

determined by the phase of the off-diagonal density matrix element (18), which in turn is given by the phase of the Hamiltonian matrix elements  $t_1$  and  $t_2$  that scatter particles between the two condensates. We can easily confirm that this result is properly gauge covariant.<sup>4</sup>

The single-particle states  $\phi_i$  are eigenstates of the (fragmented) one-body density matrix  $\hat{\rho}_0$ , and are only defined to within arbitrary phase factors. All physical observables must therefore be unchanged if each  $\phi_i$  is multiplied by  $e^{i\alpha_i}$ . It is easy to follow these phases through our calculations. The hopping matrix elements transform as  $t_1 \rightarrow t_1 e^{i(\alpha_1 - \alpha_2)}$  and  $t_2 \rightarrow t_2 e^{2i(\alpha_1 - \alpha_2)}$ , so that  $\chi \rightarrow \chi + \alpha_1 - \alpha_2$ . At the end of the day, the unique condensate (20) becomes

$$\begin{aligned} \phi_g(\mathbf{r}) &\rightarrow c_1 [e^{i\alpha_1} \phi_1(\mathbf{r})] + e^{i(\chi + \alpha_1 - \alpha_2)} [c_2 e^{i\alpha_2} \phi_2(\mathbf{r})] \\ &= e^{i\alpha_1} \phi_g(\mathbf{r}). \end{aligned} \quad (21)$$

The arbitrary phases  $\alpha_i$  are only reflected in the overall phase of  $\phi_g$  (which itself is only defined up to an overall phase). The *relative* phase of  $\phi_g(\mathbf{r})$  between any two points  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are invariants. The superfluid velocity, which is proportional to the gradient of the phase, is also invariant. Thus the phase of the off-diagonal one-body density matrix element (proportional to  $\langle B \rangle$ ) is a gauge-covariant representation of the relative phase between two condensates.

**Relative phase of previously isolated condensates.** We can use a similar approach to analyse Anderson's *gedankenexperiment*<sup>10</sup> in which two independently created condensates  $\phi_L$  and  $\phi_R$  are placed in contact. Before contact is established, the many-body state of the combined system is a simple product of states – *i.e.*, a “fragmented condensate” – that we can denote  $|q = 0\rangle$ . Since the off-diagonal element  $\langle q = 0 | b_L^\dagger b_R | q = 0 \rangle$  of the density matrix is zero, the relative phase between the two condensates is the phase of the complex number zero, which is ill-defined.

For *gedanken* purposes, let us assume that the two independent condensates are identical, with equal chemical potentials. (Our discussion is easily generalized.) As shown in the previous section, we may without loss of generality choose both  $\phi_L$  and  $\phi_R$  to be real. The time evolution following the initiation of contact is governed by a Hamiltonian of the form (7), plus damping,<sup>19</sup> with  $t_2 \ll t_1$ . By time-reversal symmetry, the  $t_i$  are real, and  $\chi = 0$  or  $\pi$ ; for definiteness we assume conventional tunneling contact, with  $\chi = 0$ . In contrast to the case of spatially overlapping fragments, however, the Josephson coupling  $t_{\text{eff}}$  between two reservoirs in contact will be proportional to their contact area, and exponentially small in the energy barrier between them.<sup>25</sup>

Except for the discreteness of  $q$ , this is a familiar problem. At long times, the system ends up in a Gaussian ground state, which we have seen is simply a conventional condensate with uniform phase. Relative to this “vacuum,” the initial state  $q = 0$  is “squeezed,” with

a width  $\delta q \sim 1$  in position and  $\delta p \sim \pi$  in the conjugate momentum. The establishment of phase coherence between two previously isolated condensates is therefore equivalent to the decay of a “squeezed vacuum” in quantum optics.<sup>20</sup> For our purposes, the important feature is that due to the  $\pm q$  symmetry of the initial state and the Hamiltonian,  $\langle B^\dagger \rangle = \langle B \rangle$  for all time. The off-diagonal density matrix element is then always real, so as soon as the relative phase becomes defined, it is zero.

The experiment of Andrews *et al.*<sup>21</sup> in which two nominally identical, initially isolated condensates are allowed to expand and overlap can also be cast in this form. If the condensates are initially converging symmetrically, then  $\phi_R(z) = \phi_L(-z)^*$ , and we again find that the transfer matrix element that scatters particle between the condensates is real. This result is consistent with Naraschewski *et al.*’s analysis<sup>22</sup> of the interference fringes seen in the MIT experiment, which requires  $\chi = 0$ .

**Random vs. reproducible phases.** Javanainen and Yoo<sup>13</sup> and Castin and Dalibard<sup>14</sup> have discussed protocols in which a series of measurements is performed on the states of individual particles removed from two isolated condensates. Their elegant analyses show that the interference patterns that emerge are consistent with a well-defined phase difference between the two condensates. This phase difference, however, is arbitrary, and varies if the entire series of measurements are repeated. How can our calculation be reconciled with these results?

In the schemes of refs. 13 and 14, each measurement of the series removes a particle from the two-condensate system in a defined superposition of the original condensates  $\phi_i$ . The remaining particles are therefore left in a specific entangled many-body state that depends on the results of the measurements. In other words, a series of observations of the removed particles generates a specific perturbation  $\delta\mathcal{H}(t)$  acting on the remaining particles. This perturbation does not conserve particle number, and in effect applies a time-dependent, gauge-symmetry-breaking “ $\eta$ -field”<sup>23</sup> to the condensates.

As we have seen, the susceptibility of the state  $q = 0$  to such a perturbation is divergent with  $N$ . Thus it only takes a small perturbation (*i.e.*, a few measurements) to sculpt the state of the remaining particles into a single condensate, whose relative phase depends deterministically on the  $\delta\mathcal{H}(t)$ , and hence on the specific sequence of observations performed on the removed particles. We have shown above that when the two condensates are placed in particle-exchanging contact their coupling *also* introduces a perturbation, which reproducibly enforces a relative phase of zero. An interesting question is the manner in which this effect competes with the measurement scenarios of refs. 13 and 14.

**Acknowledgements.** I thank N. Wilkin, R. Smith, J. Gunn, D. Butts, M. Mitchell, J. Ho, J.C. Davis, D. Weiss, J. Garrison, S. Kivelson, and R. Chiao for many interesting conversations.

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- <sup>24</sup> In a straightforward extension of the analysis given here, the case of  $N_{\text{con}}$  coexisting condensates can be mapped onto an  $(N_{\text{con}} - 1)$ -dimensional harmonic oscillator, and

the unique ground state can be determined. This many-body ground state is a conventional Bose condensate with a unique condensate wavefunction. The crucial requirement is that the occupation numbers of the condensates must be macroscopic, hence the restriction to a finite number of condensates. It is an interesting question to ask whether the number of condensates  $N_{\text{con}}$  can scale in some nontrivial way with total particle number  $N$  to preserve fragmentation.

<sup>25</sup> We emphasize that the behavior of multiple spatially *overlapping* condensates (as proposed by Ref. 8, and considered in the first part of the present work) can be different from that of two spatially *separated* condensates (whose behavior when brought into contact is discussed in the second part of this paper). For separated condensates the hopping matrix elements  $t_i$  will be exponentially small in the height of the intervening energy barrier. Then  $TN$ , while formally macroscopic (*i.e.*, proportional to  $N$ ), can also be negligibly small. For overlapping condensates this behavior is not expected.

<sup>26</sup> The assumption that the condensate fragments are compressible fluids excludes the case of Bose insulators in particle-exchanging contact, for which the energy  $\langle q|\mathcal{H}|q\rangle$  would depend on  $|q|$ .

<sup>27</sup> We emphasize again that for the case of two condensates separated by a barrier,  $T$  and  $T'$  will be exponentially small in the barrier height. Thus according to the condition derived here, a “fragmented” state could then be stable even for “macroscopic”  $N$ . This is simply the statement that two sufficiently far separated reservoirs of bosons can condense independently. This behavior is distinct from the fragmentation of spatially overlapping condensates as discussed in ref. 8.